

Strong correlations and the anisotropy of acceptor states in insulating $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$

M. B. Silva Neto¹

¹*Instituto de Física, Universidade Federal do Rio de Janeiro, Caixa Postal 68528, Brasil*

We use the Green's function formalism to discuss the role of strong correlations to the spatial structure of acceptor states doped into a two-dimensional Mott-Hubbard antiferromagnetic insulator. When the scattering between doped carriers, at the nesting wave vector $\mathbf{Q} = (\pi, \pi)$, is strong enough to produce a momentum dependent scattering rate, $\Gamma_{\mathbf{k}}$, the corresponding acceptor states become spatially anisotropic. As an example, we calculate the spatial structure of an acceptor state bound to an attractive two-dimensional Dirac delta potential, for a simple form of $\Gamma_{\mathbf{k}}$. We then discuss the role of such spatial anisotropy for the understanding of an apparent discrepancy between low temperature transport data and photoemission spectra in lightly doped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$.

PACS numbers: 78.30.-j, 74.72.Dn, 63.20.Ry, 63.20.dk

The quantitative description of hopping conductance in extrinsic semiconductors relies on what is called the effective mass approximation¹. Once the band structure of the host material is known, the effective masses on top of the valence band, for acceptors, or bottom of the conduction band, for donors, can be calculated, and a Schrödinger equation for the trap potential, generated by the impurity ions on the doped carriers, is then written down². The bound states associated with the negative energy solutions to this equation correspond to localized states and, usually, the envelope function at the lowest energy state is spatially isotropic, symmetric, parity even, just like the Hydrogen atom 1s state. The Bohr radius of the bound state (or inverse effective mass) controls the exponential decay of the envelope wave function, the overlap between two spatially separated impurity states, and directly affects the hopping conductance.

Undoped cuprates, such as La_2CuO_4 , are far from being classified as extrinsic semiconductors. These insulating materials actually belong to the class of strongly correlated electron systems, and exhibit long ranged antiferromagnetic order in the ground state. Nevertheless, it has been found that, when doped with a small amount of carriers, $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, for example, exhibits metallic behavior at high temperature (albeit anomalous) already for 1% of carriers³. Furthermore, $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ also exhibits hopping conductance at low temperature, in a very similar fashion as described above. In particular, at $x = 3\%$ and $x = 4\%$, both AC⁴ and DC⁵ data are consistent with hopping transport and point towards the existence of localized acceptor states.

Contrary to the above tendency, recent angular resolved photoemission spectroscopy (ARPES) experiments in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ revealed a certain degree of "metallicity" at the same doping regime discussed above⁶, and have, as a result, been interpreted as evidence for delocalization of the charge carriers. The observation of "quasiparticle" peaks in the form of small Fermi arcs for 3% doped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ at $T = 10\text{K}$ ⁶, which according to transport should be insulating, resembles very much the full pocket structure observed in other cuprates at higher doping⁷, where the sample is (strangely) metallic. The conclusion was that, since ARPES shows "peaks" in

reciprocal (momentum) space, the associated wave function should be extended in real (coordinate) space, and not localized as suggested by hopping transport.

As an attempt to address this apparent discrepancy, A. S. Alexandrov and K. Reynolds⁸ suggested that such Fermi arcs observed with ARPES in insulating $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ could arise naturally from matrix elements when the ejected electron leaves behind a hole at *valence band tails*, formed by the hybridization of valence band and impurity states². The reasoning is actually relatively simple. While long-lived quasiparticles in a Fermi liquid have very well defined momentum states and thus give rise to sharp peaks in the ARPES spectrum, localized wave functions are written as a linear superposition of many different wave vectors, and, as a consequence, do not possess a well defined momentum state. For this reason, no peaks are to be expected in the ARPES spectrum corresponding to a bound state. For a sufficiently large envelope wave function, however, the ARPES matrix elements in reciprocal space will depend on which of the linearly combined wave vectors weigh a heavier contribution to the spectral function. For the case of cuprates, for example, it is argued, in Ref. 8, that the wave vectors close to $(\pi/2, \pi/2)$ contribute a much higher spectral weight, which then falls rapidly away from this point⁸. For this reason, bound electrons ejected from band tails are able to produce Fermi arcs in the ARPES spectrum.

A necessary condition for the Alexandrov and Reynolds idea to work is that the localized state should be anisotropic in real space⁸, being more elongated along the direction perpendicular to the Brillouin zone (B.Z.) faces, and being shorter along the direction parallel to it⁸. In this work we extend the traditional effective mass approximation to include strong correlations, and we calculate the full spatial structure of acceptor states using a phenomenological model to mimic light doping in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$. We argue that due to the presence of a nesting AF wave vector $\mathbf{Q} = (\pi, \pi)$ (in units of the lattice spacing $a = 1$) the localized states become squeezed exactly along the B.Z. faces and elongated along the so called nodal directions (along the direction perpendicular to the B.Z. faces), providing the missing ingredient to complete the Alexandrov and Reynolds analysis.

We begin by reviewing the effective mass approximation for the calculation of acceptor/donor states in extrinsic semiconductors². The effective mass tensor, $m_{\alpha\beta}^*$, is defined as $(m_{\alpha\beta}^*)^{-1} = \partial^2 \varepsilon(\mathbf{k}) / \partial k_\alpha \partial k_\beta$, where $\varepsilon(\mathbf{k})$ is the quasiparticle dispersion close to the bottom of the conduction band (for donors) or top of the valence band (for acceptors) located at the i -th pocket. In case the effective mass tensor is diagonal, but with different components, m_{\parallel}^* and m_{\perp}^* , the time-independent Schrödinger equation for the localized wave function $\psi^i(\mathbf{r})$ reads

$$\left[- \left(\frac{\hbar^2 \nabla_{\parallel}^2}{2m_{\parallel}^*} + \frac{\hbar^2 \nabla_{\perp}^2}{2m_{\perp}^*} \right) + V(\mathbf{r}) + U(\mathbf{r}) \right] \psi^i(\mathbf{r}) = E \psi^i(\mathbf{r}), \quad (1)$$

where $\nabla_{\perp} = \partial/\partial z$, $\nabla_{\parallel} = (\partial/\partial x, \partial/\partial y)$, $V(\mathbf{r})$ is the periodic potential provided by the lattice, and $U(\mathbf{r})$ is the trap potential felt by the doped carriers and provided by an impurity at the origin of the coordinate system. For large enough bound states, when the localization length is of the order of several lattice spacings, one can write

$$\psi^i(\mathbf{r}) = F^i(\mathbf{r}) \phi^i(\mathbf{k}^i, \mathbf{r}), \quad (2)$$

where $F^i(\mathbf{r}) \sim e^{-r/\xi^i}$ is usually an exponentially decaying envelope wave function with localization length ξ^i at the i -th pocket and, according to Bloch's theorem, $\phi^i(\mathbf{k}^i, \mathbf{r}) = e^{i\mathbf{k}^i \cdot \mathbf{r}} u_{\mathbf{k}^i}(\mathbf{r})$, where $u_{\mathbf{k}^i}(\mathbf{r})$ is a periodic function with minimum at \mathbf{k}^i . Following Kohn and Luttinger (KL)⁹, each one of the $\mu = 1 \dots N$ degenerate (from different pockets) localized states are generally written as

$$\Psi_{\mu} = \sum_{i=1}^N \alpha_{\mu}^i \psi^i(\mathbf{r}) = \sum_{i=1}^N \alpha_{\mu}^i F^i(\mathbf{r}) \phi^i(\mathbf{k}^i, \mathbf{r}), \quad (3)$$

where α_{μ}^i are N -dimensional vectors determined by point group symmetry carrying the information about the symmetries of the wave functions. We define $\gamma = m_{\perp}^*/m_{\parallel}^*$, and $F^i(\mathbf{r}) \sim e^{-r/\xi^i}$ can be classified as isotropic 3-D, $\gamma = 1$, in which case $r = \sqrt{x^2 + y^2 + z^2}$, or extremely adiabatic 2-D, $\gamma \rightarrow 0$, in which case $r = \sqrt{x^2 + y^2}$.

It has long been acknowledged that, to a very good extent, the physics of lightly doped cuprates is well captured by the $t - t' - t'' - J$ model¹⁰, which includes not only nearest neighbor hopping, t , but also second neighbor hoppings, t' and t'' , for holes doped into a two-dimensional antiferromagnet with superexchange J . At a very small concentration, the Fermi surface for the added holes correspond to four, nearly two-dimensional hole pockets centered at the wave vectors $\mathbf{k}_0 = (\pm\pi/2, \pm\pi/2)$ in the magnetic B.Z., as can be seen in Fig. 1a). This is consistent with band structure calculations, as well as ARPES data⁷, and the two-dimensionality of the Fermi surface results from the huge effective along the direction perpendicular to the CuO₂ planes (or parallel to the c -axis), $m_{\perp}^* \gg m_{\parallel}^*$, where m_{\parallel}^* is the planar effective mass. The above large effective mass anisotropy drives

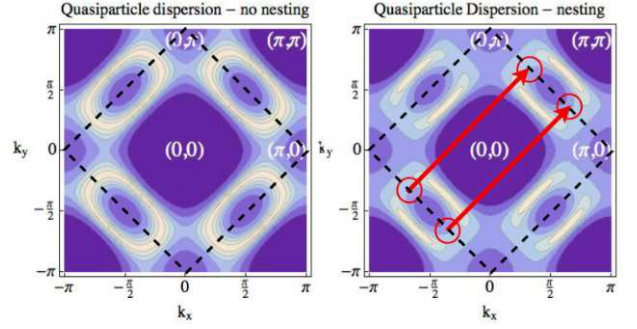


FIG. 1: (Color online) Evolution of the quasiparticle spectrum: a) (left) fully coherent hole-like Fermi pockets⁷, located at $\mathbf{k}_0 = (\pm\pi/2, \pm\pi/2)$ in the magnetic B. Z.; b) (right) additional scattering at the nesting antiferromagnetic wave vector¹², $\mathbf{Q} = (\pi, \pi)$, and the *hot spots* along the magnetic B.Z. faces (effect of a \mathbf{k} -dependent scattering rate $\Gamma_{\mathbf{k}}$).

the system into the extreme adiabatic limit discussed above, $\gamma \rightarrow 0$. Self consistent Born approximation for the $t - t' - t'' - J$ model has also determined that, at the very top of the valence band, the pockets are nearly circular, with equal effective masses along the magnetic B.Z. faces and diagonals, or orthorhombic (a, b) axis, and thus we can set $m_a^* \simeq m_b^* = m_{\parallel}^*$. In this case

$$F(\mathbf{r}) \sim e^{-r/\xi}, \quad (4)$$

where $r = \sqrt{x^2 + y^2}$ and $\xi \sim 1/m_{\parallel}^*$. Such large effective mass anisotropy, $m_{\perp}^* \gg m_{\parallel}^*$ is consistent with the large resistivity anisotropy in these materials⁵, $\rho_c/\rho_{ab} \sim 10^3$.

However, a 2D isotropic wave function is not consistent with neither the ARPES response for very lightly doped La_{2-x}Sr_xCuO₄ nor with the AC and DC transport measurements at low temperature, in the hopping regime, where the knowledge of the precise shape of the localized state turns out to be crucial. These experiments have revealed that, besides the perpendicular anisotropy discussed above, $m_{\perp}^*/m_{\parallel}^* \gg 1$, an additional in-plane anisotropy is necessary to account for the different infrared absorption spectra observed along the two orthorhombic directions in La_{2-x}Sr_xCuO₄⁴. In what follows, we shall argue that, even more important than the anisotropy caused by spiral correlations considered by V. Kotov and O. Sushkov in Ref. 11, is the anisotropy coming from strong correlations, in the form of a momentum dependent scattering rate^{12,13}. This will force us to extend the usual effective mass approximation, used in Eq. (1), in order to incorporate such nontrivial effect.

On general grounds, we shall assume that the original quasiparticle dispersion of the noninteracting, $J = 0$, problem, the $t - t' - t''$ model, have the pocket like structure at $\mathbf{k}_0 = (\pm\pi/2, \pm\pi/2)$ shown in Fig. 1a). For $J \neq 0$, in turn, short wavelength antiferromagnetic fluctuations, at low temperature and near half-filling, cause the enhancement of the quasiparticle scattering at the ordering wave vector¹², see Fig. 1b). The presence of such *hot*

spots produces, in turn, a momentum dependent scattering rate (or inverse quasiparticle lifetime)¹³, which provides us with an important source of anisotropy.

For simplicity, let us consider the problem of a hole under the influence of an attractive 2D-delta potential¹⁴. According to the usual effective mass approximation, the envelope wave function $F(\mathbf{r})$ can be obtained from

$$\left[-\frac{\hbar^2 \nabla^2}{2m_{\parallel}^*} + U(\mathbf{r}) \right] F(\mathbf{r}) = E F(\mathbf{r}), \quad (5)$$

where

$$U(\mathbf{r}) = -g \frac{\delta(\mathbf{r} - \mathbf{r}_0)}{r} \quad (6)$$

is an attractive δ -potential that traps, with strength g , a hole around an impurity ion at the origin. We shall be interested in the solutions to this equation for \mathbf{r} larger than the cutoff \mathbf{r}_0 . Using the Fourier transform

$$F(\mathbf{r}) = \int \frac{d^2 \mathbf{k}}{(2\pi)^d} e^{-i\mathbf{k} \cdot \mathbf{r}} f(\mathbf{k}), \quad (7)$$

the equation becomes

$$\int \frac{d^2 \mathbf{k}}{(2\pi)^d} \left[\frac{\hbar^2 \mathbf{k}^2}{2m_{\parallel}^*} - E \right] e^{-i\mathbf{k} \cdot \mathbf{r}} f(\mathbf{k}) = g \frac{\delta(\mathbf{r} - \mathbf{r}_0)}{r} F(\mathbf{r}). \quad (8)$$

We now multiply the whole equation by $(2\pi)^2 e^{i\mathbf{q} \cdot \mathbf{r}}$, and integrate over \mathbf{r} to obtain

$$f(\mathbf{q}) = \frac{4\pi^2 g_0 F(r_0)}{\varepsilon(\mathbf{q}) + \varepsilon_B} = g_0 \frac{f(r_0)}{\varepsilon(\mathbf{q}) + \varepsilon_B}, \quad (9)$$

where we defined $g_0 = g/r_0$, $f(r_0) = 4\pi^2 F(r_0)$, and $\varepsilon(\mathbf{q}) = \hbar^2 \mathbf{q}^2 / 2m_{\parallel}^*$, is the dispersion in the effective mass approximation. Here we have used, as the negative energy (bound state) solution, $-E = \varepsilon_B = \hbar^2 \kappa^2 / 2m_{\parallel}^*$, with $\kappa = 1/\xi$ playing the role of inverse localization length ξ . We recognize Eq. (9) as a particular case of the more generic Bethe-Salpeter equation for a potential $U(\mathbf{r})$

$$f(\mathbf{q}) = -\frac{4\pi^2}{\varepsilon(\mathbf{q}) + \varepsilon_B} \int \frac{d^2 \mathbf{k}'}{(2\pi)^2} \tilde{U}(\mathbf{k}' - \mathbf{q}) f(\mathbf{k}'), \quad (10)$$

with $\tilde{U}(\mathbf{k})$ being, as usual, the Fourier transform of $U(\mathbf{r})$.

The result presented in (9) is the exact solution to the equation (5) in which all wave vector are treated on equal footing. In particular, the term $\hbar^2 \nabla^2 / 2m_{\parallel}^*$ is isotropic and results from the nearly perfect circular shape of the hole pockets in lightly doped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$. For this reason, $f(\mathbf{q})$ depends only on \mathbf{q}^2 and the resulting envelope function $F(\mathbf{r})$ is also isotropic. In order to introduce the momentum dependence of the scattering rate¹², Γ_k , a quantity that is related to the quasiparticles spectral function and which does not appear in (5), we will make

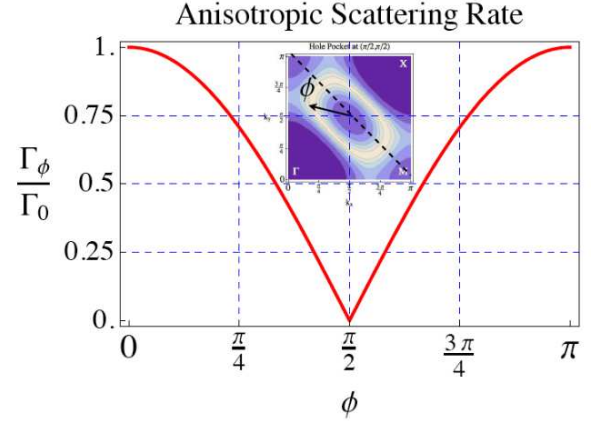


FIG. 2: (Color online) Anisotropic scattering rate Γ_ϕ (red solid line) as a function ϕ . Inset: ϕ is the angle between the wave vector \mathbf{q} (black solid arrow) and the magnetic B.Z. face (black dashed line). At the hot spots, $\phi = 0, \pi$, the scattering is maximal, while at the nodal direction, $\phi = \pi/2$, it is minimal¹³.

use of the Green's functions formalism, and its spectral representation. We perform a Stieltjes transform to write

$$G(\mathbf{q}, \omega = 0) = \frac{1}{\varepsilon(\mathbf{q}) + \varepsilon_B} = \int_{-\infty}^{\infty} dE \frac{A(\mathbf{q}, E)}{E + \varepsilon_B}, \quad (11)$$

where the spectral function $A(\mathbf{q}, E)$ is, for such strongly correlated electron system, given by

$$A(\mathbf{q}, E) = \frac{Z_{\mathbf{q}}}{\pi} \frac{\Gamma_{\mathbf{q}}}{(E - \varepsilon(\mathbf{q}))^2 + \Gamma_{\mathbf{q}}^2} + A_{inc}(\mathbf{q}, E), \quad (12)$$

where $Z_{\mathbf{q}}$ is the quasiparticle weight, $\Gamma_{\mathbf{q}}$ is the momentum dependent scattering rate, and A_{inc} is the incoherent (or multiparticle) part of the spectrum. For a weakly interacting system, a Fermi liquid, where $\Gamma_{\mathbf{q}} = \Gamma_0 \rightarrow 0$, one ends up with $A(\mathbf{q}, E) = Z_{\mathbf{q}} \delta(E - \varepsilon(\mathbf{q})) + A_{inc}(\mathbf{q}, E)$.

Since the nesting is strongest for the points where the pockets intersects the B.Z. faces, we can, without loss of generality, consider the phenomenological formula

$$\Gamma_{\mathbf{q}} = \Gamma_0 |\cos(\phi)|, \quad (13)$$

where ϕ is the angle between the wave vector \mathbf{q} , centered at a given pocket, and the B.Z. face. This simple form of the scattering rate produces larger widths for the spectral lines along the B.Z. faces, the hot spots at $\phi = 0, \pi$, very small widths along the nodal directions, $\phi = \pi/2$ (see Fig. 2), and is consistent with the results from Ref. 13.

For calculating bound states, it is enough to keep only the coherent part of the spectrum, defined as $A_{coh}(\mathbf{q}, E) = A(\mathbf{q}, E) - A_{inc}(\mathbf{q}, E)$, and thus we write

$$F(\mathbf{r}) = g_0 f(0) \int \frac{d^2 \mathbf{q}}{(2\pi)^2} \int dE \frac{e^{-i\mathbf{q} \cdot \mathbf{r}}}{E + \varepsilon_B} A_{coh}(\mathbf{q}, E). \quad (14)$$

We now make the following approximations. We use explicitly that $Z_{\mathbf{q}} = Z_0$, that is, the quasiparticle weight is

weakly momentum dependent at low doping, and we use explicitly the angular dependence of the scattering rate, $\Gamma_{\mathbf{q}} = \Gamma_{\phi}$. We evaluate this integral by closing a contour in the upper half plane and use the residue theorem

$$F(\mathbf{r}) = g_0 f(r_0) \mathcal{Z}_0 \int \frac{d^2 \mathbf{q}}{(2\pi)^2} e^{-i\mathbf{q} \cdot \mathbf{r}} \frac{\varepsilon(\mathbf{q}) + \varepsilon_B}{(\varepsilon(\mathbf{q}) + \varepsilon_B)^2 + \Gamma_{\phi}^2}, \quad (15)$$

where we have used explicitly that $\mathcal{Z}_{\mathbf{q}} = \mathcal{Z}_0$ and $\Gamma_{\mathbf{q}} = \Gamma_{\phi}$. Notice that in the limit where $\Gamma_{\phi} \rightarrow 0$ and $\mathcal{Z}_0 \rightarrow 1$ the above equation reduces to the result obtained in (9).

Before performing the angular integration, we must recall that, while ϕ is the angle between \mathbf{q} and the B.Z.

face, the angle θ that appears in $\mathbf{q} \cdot \mathbf{r} = qr \cos \theta$, is the angle between \mathbf{q} and \mathbf{r} . So, if we define as φ the angle between \mathbf{r} and the B.Z. face at a given pocket, we end up with $\theta = \phi - \varphi$. The complete solution to the bound state problem can be finally presented. We approximate $\Gamma_{\phi} \ll \varepsilon_B$, and write $F_{\varphi}(\mathbf{r}) = F_0(\mathbf{r}) + \delta F_{\varphi}(\mathbf{r})$, where

$$F_0(\kappa, \mathbf{r}) = g_0 f(r_0) \mathcal{Z}_0 \frac{m_{\parallel}^*}{\pi \hbar^2} K_0(\kappa r), \quad (16)$$

is the unperturbed ($\Gamma_0 = 0$) isotropic (φ -independent) contribution to the wave function, while the perturbation (and source of anisotropy in φ) becomes

$$\delta F_{\varphi}(\kappa, \mathbf{r}) = g f(r_0) \mathcal{Z}_0 \Gamma_0^2 \frac{2(m_{\parallel}^*)^2}{\kappa \hbar^4} \left\{ \frac{2(2 - \kappa^2 r^2 K_0(\kappa r)) \cos(2\varphi) - \kappa r K_1(\kappa r) (\kappa^2 r^2 + (4 + \kappa^2 r^2) \cos(2\varphi))}{2\kappa^3 r^2} \right\}, \quad (17)$$

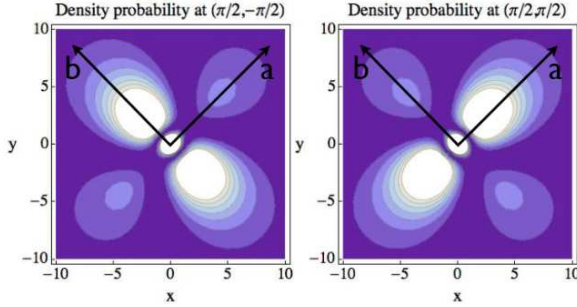


FIG. 3: (Color online) Density plot of the amplitude probability for the envelope wave function $F(\mathbf{r})$, at the two nonequivalent pockets: a) (left) $(\pi/2, -\pi/2)$; and b) (right) $(\pi/2, \pi/2)$. The axis a and b are the orthorhombic axis.

where K_0 and K_1 are modified Bessel functions of the second kind and, from its definition, φ is given by $\varphi = \arctan[(x \mp y)/(x \pm y)]$, for the pockets centered at $(\pi/2, \pm\pi/2)$, see Fig. 3. We see that, as required by

Alexandrov and Reynolds⁸, the spatial structure of the acceptor state is such that the envelope wave function is elongated exactly along the nodal directions, or perpendicular to the B.Z. faces, and squeezed along the directions parallel to the B.Z. faces.

We have extended the traditional effective mass approximation² to include the effects from strong correlations, reflected in the anisotropy of the quasiparticle scattering rate¹², $\Gamma_{\mathbf{k}}$ (or inverse quasiparticle lifetime). Using the Green's function method, and its spectral representation, we were able to calculate the full structure of an acceptor state trapped by a simple two-dimensional δ -potential, used to mimic the problem of lightly doping a Mott-Hubbard antiferromagnetic insulator. Our results provide the missing ingredient to the Alexandrov and Reynolds analysis⁸, which bridges the gap between low temperature transport^{4,5} and ARPES⁶ data.

The author acknowledges discussions with A. Alexandrov, G. Blumberg, R. Capaz, A. Chernyshev, B. Koiller, and O. Sushkov.

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